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Parallel Implementation of the Self-Consistent-Charge Density-Functional-Based Tight-Binding

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The density-functional-based tight-binding method with charge-selfconsistency (SCC-DFTB) has been applied to a variety of problems in the fields of solids, surfaces, inorganic clusters and even biological molecules. This fast and efficient method has proved to be very accurate, results are usually in very good agreement with fully self-consistent DFT results.
The method has been implemented for parallel computers based on MPI and Scalapack and was tested on various hardware including the T3E and PC-based distributed-memory computers. We present details about the performance and scaling behaviour and demonstrate applications of the parallel code.